Claims

What is claimed is:

1. A method for monitoring enantiomeric excess of a plurality of chiral molecules participating in a chemical reaction comprising:
   a means for obtaining a plurality of Fourier transform vibrational circular dichroism spectra and Fourier transform absorption spectra in the mid infrared region of a chemical solution when a chemical reaction is occurring in said chemical solution; a means for ordering said plurality of Fourier transform vibrational circular dichroism and absorption spectra as a function of time of collection of spectra; a means for analyzing said Fourier transform vibrational circular dichroism spectra and absorption to determine simultaneously the concentration and enantiomeric excess of each chiral molecule as a function of time.

2. A method for monitoring enantiomeric excess of a plurality of chiral molecules participating in a chemical reaction comprising:
   a means for obtaining a plurality of Fourier transform vibrational circular dichroism spectra and Fourier transform absorption spectra in the near infrared region of a chemical solution when a chemical reaction is occurring in said chemical solution; a means for ordering said plurality of Fourier transform vibrational circular dichroism and absorption spectra as a function of time of collection of spectra; a means for analyzing said Fourier transform vibrational circular dichroism spectra and absorption to determine simultaneously the

concentration and enantiomeric excess of each chiral molecule as a function of time.

3. A method as claimed in claim 1 wherein said chemical solution is monitored by means of a flow cell.

4. A method as claimed in claim 2 wherein said chemical solution is monitored by means of a flow cell.

5. A method as claimed in claim 1 wherein said chemical solution is monitored by means of a fiber-optically-coupled accessory with or without a flow cell.

6. A method as claimed in claim 2 wherein said chemical solution is monitored by means of a fiber-optically-coupled accessory with or without a flow cell.

7. A method for determining the enantiomeric excess of chiral molecule in a solution including:

obtaining an actual concentration coefficient from an IR spectrum for the solution;

obtaining the apparent concentration coefficient of the VCD spectrum for the solution;

dividing the apparent concentration coefficient of the VCD spectrum by the actual concentration coefficient from IR spectrum to obtain a %EE.

8. The method of claim 7 wherein the steps of obtaining an IR spectrum, and/or coefficients, and obtaining a VCD spectrum, and/or coefficients are performed simultaneously.

9. The method for monitoring the enantiomeric excess of molecules in a reaction chamber, including:

providing a reaction chamber to contain the molecules;

providing an instrument for producing both an IR spectrum and a VCD spectrum of the molecules in the reaction chamber;

using the instrument to obtain an IR spectrum and the VCD spectrum of the molecules in the reaction chamber;

obtaining the actual concentration coefficients of each species from the IR spectrum and the apparent coefficients of each species from the VCD spectrum;

dividing the apparent concentration coefficient of each species present in the VCD spectrum by the corresponding actual concentration coefficient of each species in the IR spectrum,

thereby obtaining the %EE of each species present in the reaction chamber during the course of the reaction.

10. The method of claim 9, further including providing a fiberoptic pathway between the reaction chamber and the instrument.

11. The method of claim 9, further including using a partial least squares analysis, to determine the actual concentration coefficients of the IR spectrum and the apparent concentration coefficients of the VCD spectrum by comparison to the IR spectrum and the VCD spectrum of the molecule at known concentrations.

12. The method of claim 9, further including using a chemometrics analysis, to determine the actual concentration coefficients of the IR spectrum and the

apparent concentration coefficients of the VCD spectrum by comparison to the IR spectrum and the VCD spectrum of the molecule at known concentrations.

13. The method of claim 9, further including a flow cell connected to the reaction chamber and positioning the instrument for producing both the IR spectrum and the VCD spectrum in proximity to the flow cell, so that the spectra are produced by sampling the molecules in the flow cell.

14. The method of claim 9, wherein the temperature and pressure of the reaction chamber environment are controllable, and wherein the %EE information for a particular molecule of interest is used to control the temperature, pressure and/or other conditions of the reaction chamber.